

09/759,633

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	DEC 08	INPADOC: Legal Status data reloaded
NEWS	5	SEP 29	DISSABS now available on STN
NEWS	6	OCT 10	PCTFULL: Two new display fields added
NEWS	7	OCT 21	BIOSIS file reloaded and enhanced
NEWS	8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS	9	NOV 24	MSDS-CCOHS file reloaded
NEWS	10	DEC 08	CABA reloaded with left truncation
NEWS	11	DEC 08	IMS file names changed
NEWS	12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS	13	DEC 09	STN Entry Date available for display in REGISTRY and CA/CAPLUS
NEWS	14	DEC 17	DGENE: Two new display fields added
NEWS	15	DEC 18	BIOTECHNO no longer updated
NEWS	16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS	17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS	18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS	19	DEC 22	ABI-INFORM now available on STN
NEWS	20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAPLUS
NEWS	22	FEB 05	German (DE) application and patent publication number format changes
NEWS	23	MAR 03	MEDLINE and LMedline reloaded
NEWS	24	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	25	MAR 03	FRANCEPAT now available on STN
NEWS EXPRESS			MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
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NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

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FILE 'HOME' ENTERED AT 11:59:35 ON 18 MAR 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:59:42 ON 18 MAR 2004

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STRUCTURE FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8

DICTIONARY FILE UPDATES: 17 MAR 2004 HIGHEST RN 664302-53-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\09759633.str

L1 STRUCTURE UPLOADED

=> s l1 ful

FULL SEARCH INITIATED 12:00:06 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 407 TO ITERATE

100.0% PROCESSED 407 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

L2 25 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

155.42

155.63

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FILE 'CAPLUS' ENTERED AT 12:00:12 ON 18 MAR 2004  
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FILE COVERS 1907 - 18 Mar 2004 VOL 140 ISS 12  
FILE LAST UPDATED: 17 Mar 2004 (20040317/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12  
L3

10 L2

=> d 13 ibib hitstr abs 1-10

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:526050 CAPLUS  
DOCUMENT NUMBER: 135:107149  
TITLE: Synthesis, antibacterial activity and RNA polymerase inhibition of phenylamidine derivs.  
INVENTOR(S): Li, Leping; Chen, Xiaoqui; Fan, Pingchen; Mihalic, Jeffrey Thomas; Cutler, Serena  
PATENT ASSIGNEE(S): Tularik Inc., USA  
SOURCE: PCT Int. Appl., 104 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001051456	A2	20010719	WO 2001-US1219	20010112
WO 2001051456	A3	20011220		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002045749	A1	20020418	US 2001-759633	20010112
EP 1246795	A2	20021009	EP 2001-914329	20010112
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

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IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
JP 2003519676 T2 20030624 JP 2001-551838 20010112  
PRIORITY APPLN. INFO.: US 2000-175892P P 20000113  
WO 2001-US1219 W 20010112

OTHER SOURCE(S): MARPAT 135:107149

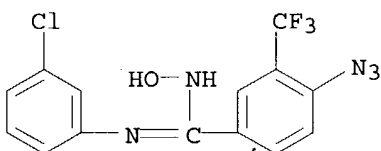
IT 350486-82-7P 350486-84-9P 350486-86-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(synthesis, antibacterial activity and RNA polymerase inhibition of phenyl- and heterocyclylhydroxyamidine derivs.)

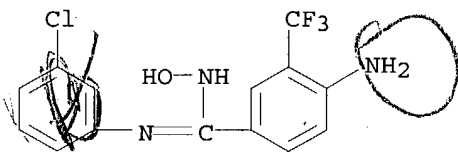
RN 350486-82-7 CAPLUS

CN Benzenecarboximidamide, 4-azido-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



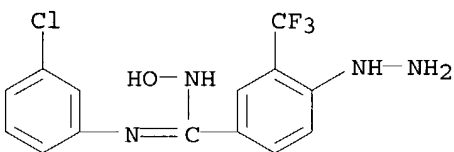
RN 350486-84-9 CAPLUS

CN Benzenecarboximidamide, 4-amino-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350486-86-1 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-hydrazino-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT 350487-08-0P 350487-09-1P 350487-13-7P

350487-14-8P 350487-15-9P 350487-18-2P

350487-19-3P 350487-20-6P 350487-22-8P

350487-25-1P 350487-26-2P 350487-31-9P

350487-96-6P 350487-97-7P 350487-98-8P

350487-99-9P

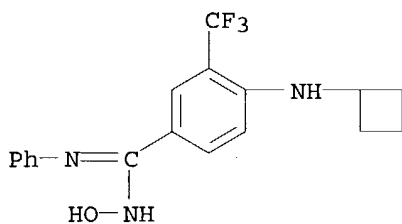
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

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BIOL (Biological study); PREP (Preparation); USES (Uses)  
(synthesis, antibacterial activity and RNA polymerase inhibition of  
phenyl- and heterocyclhydroxyamidine derivs.)

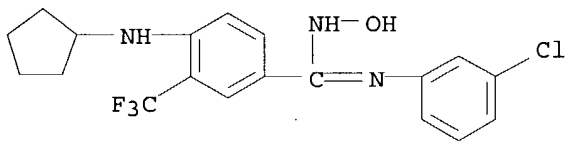
RN 350487-08-0 CAPLUS

CN Benzenecarboximidamide, 4-(cyclobutylamino)-N-hydroxy-N'-phenyl-3-  
(trifluoromethyl)- (9CI) (CA INDEX NAME)



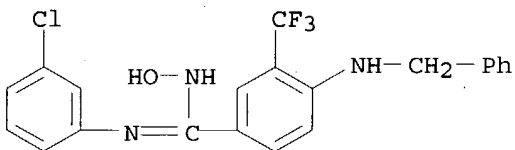
RN 350487-09-1 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopentylamino)-N'-hydroxy-  
3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



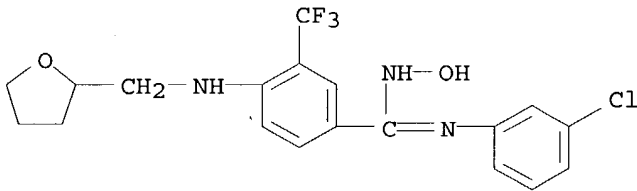
RN 350487-13-7 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-  
[(phenylmethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-14-8 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[tetrahydro-2-  
furanyl)methyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

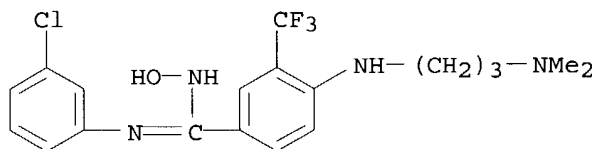


RN 350487-15-9 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[[3-

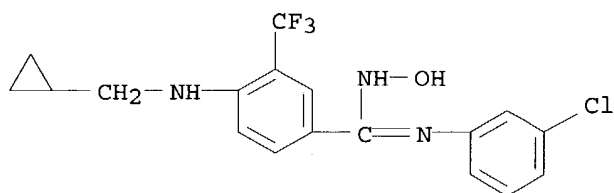
09/759,633

(dimethylamino)propyl]amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



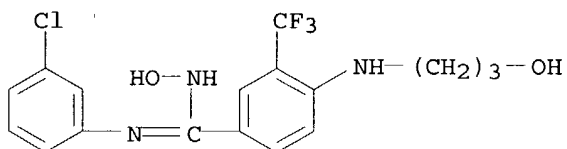
RN 350487-18-2 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-[(cyclopropylmethyl)amino]-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



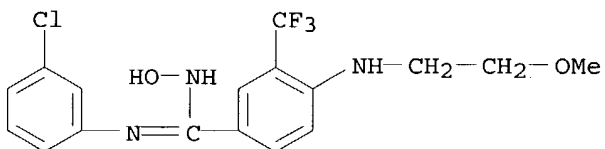
RN 350487-19-3 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(3-hydroxypropyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-20-6 CAPLUS

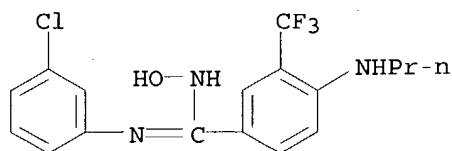
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-methoxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-22-8 CAPLUS

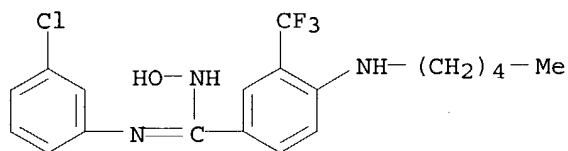
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(propylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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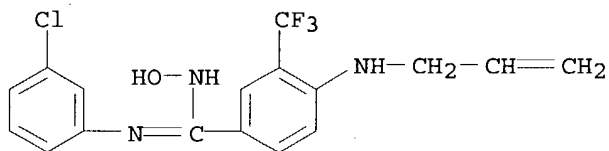
RN 350487-25-1 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(pentylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



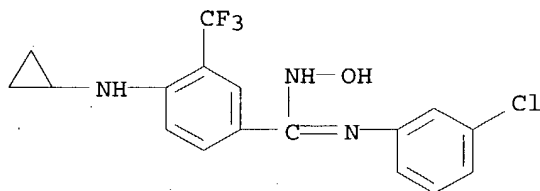
RN 350487-26-2 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-(2-propenylamino)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



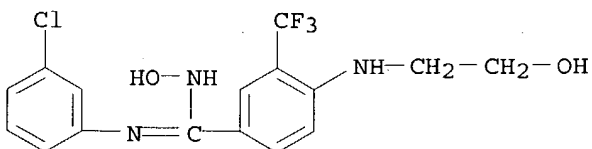
RN 350487-31-9 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-4-(cyclopropylamino)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 350487-96-6 CAPLUS

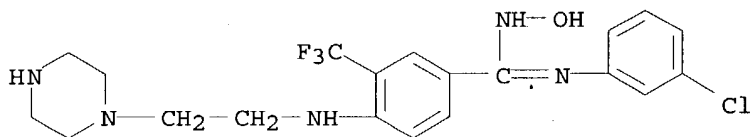
CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[(2-hydroxyethyl)amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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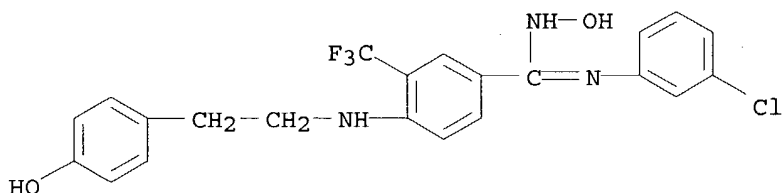
RN 350487-97-7 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[2-(1-piperazinyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



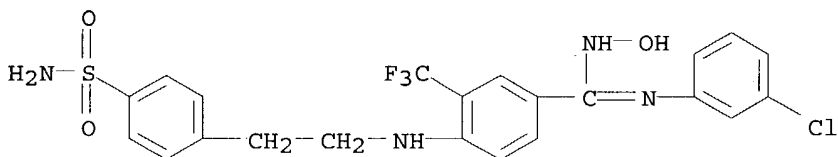
RN 350487-98-8 CAPLUS

CN Benzenecarboximidamide, N-(3-chlorophenyl)-N'-hydroxy-4-[[2-(4-hydroxyphenyl)ethyl]amino]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

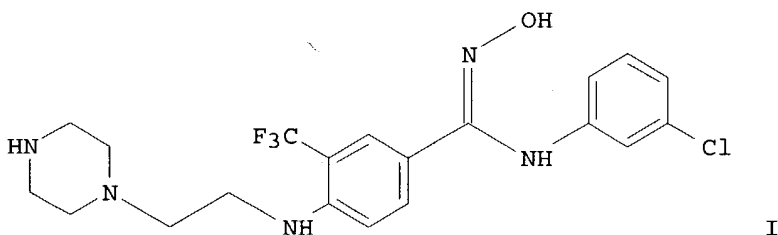


RN 350487-99-9 CAPLUS

CN Benzenecarboximidamide, 4-[[2-[4-(aminosulfonyl)phenyl]ethyl]amino]-N-(3-chlorophenyl)-N'-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



GI



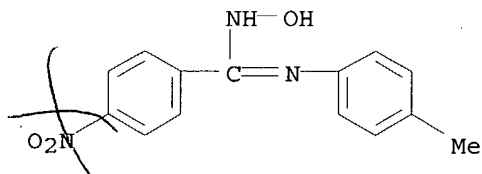
I

AB Synthesis of hydroxyamidines, e.g. (I) and related compds. are disclosed which are suitable as antibacterial agents by their inhibition of RNA polymerase. Antibacterial activity against *S. aureus* and *E. coli* are given.



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L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:276393 CAPLUS  
DOCUMENT NUMBER: 133:73985  
TITLE: A convenient synthesis of 3,4-disubstituted-1,2,4-thiadiazole-5(4H)-thiones  
AUTHOR(S): Agirbas, Hikmet; Kahraman, Kazim  
CORPORATE SOURCE: Department of Chemistry, Kocaeli University, Izmit, 41300, Turk.  
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1998), 134/135, 381-389  
CODEN: PSSLEC; ISSN: 1042-6507  
PUBLISHER: Gordon & Breach Science Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 2630-07-1, N-Hydroxy-N'-(4-methylphenyl)-4-nitrobenzenecarboximidamide  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of thiadiazolethiones by rearrangement of oxadiazolethione intermediates)  
RN 2630-07-1 CAPLUS  
CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA INDEX NAME)



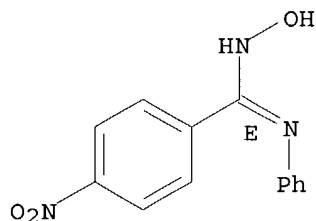
AB 3,4-Disubstituted-1,2,4-oxadiazole-5(4H)-ones were obtained from the reaction of substituted amide oximes with Et chloroformate. These compds. were treated with P2S5 to give corresponding 1,2,4-oxadiazole-5-thiones. Rearrangement of 1,2,4-oxadiazole-5-thiones, catalyzed by metallic copper, yielded 1,2,4-thiadiazole-5-ones. The reaction of 1,2,4-thiadiazole-5-ones with P2S5 gave 1,2,4-thiadiazole-5-thiones.  
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1995:908286 CAPLUS  
DOCUMENT NUMBER: 124:102365  
TITLE: Crystal and molecular structure of N-phenyl-4-nitrobenzamidoxime  
AUTHOR(S): Buzykin, B. I.; Dokuchaev, A. S.; Kharitonova, O. A.  
CORPORATE SOURCE: A. E. Arbuzov Inst. Org. Phys. Chem., Russian Acad. Sci., Kazan, 420083, Russia  
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995), (8), 1516-19  
CODEN: IASKEA  
PUBLISHER: Nauka  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
IT 172540-77-1  
RL: PRP (Properties)  
(crystal structure of)  
RN 172540-77-1 CAPLUS

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CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



AB An x-ray study of N-phenyl-4-nitrobenzamidoxime (1) was performed. Crystallog. data and atomic coordinates are given. Two crystallog. independent mols. have a planar Z-configuration of amidoxime with s-trans-conformation of these fragments related to =N-O and C-N(H) bonds. Intramol. NH...O bond is observed. Rotation angle of nitrophenyl and Ph rings related to amidoxime plane [ONCN] is -57 and -32° in 1A and -38 and -22° in 1B correspondingly. Rotation around C(1)-N(2) bond is -28 (1A) and -35° (1B). 1A and 1B mols. form oxime dimers in crystals due to two intermol. H-bond =N...(HO)', dimers forming double chains due to two more H-bonds NH...(O2N).

L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:128321 CAPLUS

DOCUMENT NUMBER: 116:128321

TITLE: Reaction of triethyl orthoformate with mono-substituted amidoximes

AUTHOR(S): Andrianov, V. G.; Ereemeev, A. V.

CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(8), 1604-7  
CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

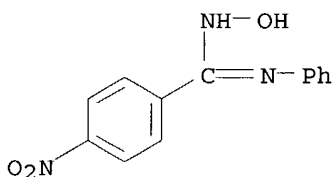
LANGUAGE: Russian

IT 57767-04-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with tri-Et orthoformate)

RN 57767-04-1 CAPLUS

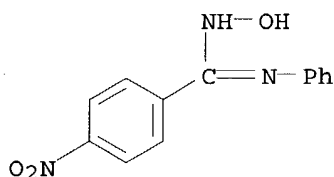
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



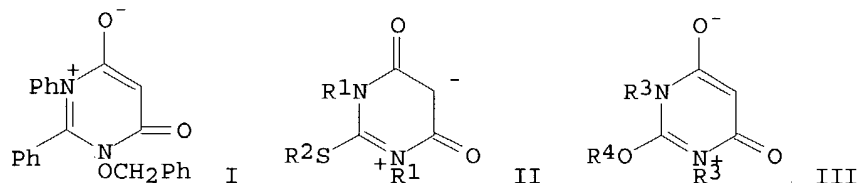
AB The reaction of 4-O2NC6H4C(:NOH)NHR (I; R = Me, Et, Ph) with CH(OEt)3 gave 4-O2NC6H4C(:NO2CNHR)NHR in 33-38% yield. I in turn were prepared from 4-O2NC6H4CCl:NOH and RNH2.

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L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1978:62359 CAPLUS  
DOCUMENT NUMBER: 88:62359  
TITLE: Syntheses of heterocycles, CCVII. Mesoionic  
pyrimidines and thiazines  
AUTHOR(S): Ziegler, Erich; Steiger, Wilfried; Strangas, Charilaos  
CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, Austria  
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische  
Chemie, Organische Chemie (1977), 32B(10), 1204-8  
CODEN: ZNBAD2; ISSN: 0340-5087  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
IT 57767-04-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with carbon suboxide)  
RN 57767-04-1 CAPLUS  
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX  
NAME)



GI

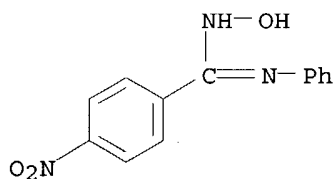


AB CH<sub>2</sub>(CO<sub>2</sub>N:CRNHPh)<sub>2</sub> (R = 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 3-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 2-ClC<sub>6</sub>H<sub>4</sub>) were obtained by treating HON:CRNHPh with C<sub>3</sub>O<sub>2</sub>. PhCH<sub>2</sub>ON:CPhNHPh similarly gave the pyrimidinone I. II (R<sub>1</sub> = Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, 2-MeC<sub>6</sub>H<sub>4</sub>; R<sub>2</sub> = Me, Et) were similarly obtained from R<sub>1</sub>N:C(SR<sub>2</sub>)NHR<sub>1</sub> and III (R<sub>3</sub> = cyclohexyl, Ph, 4-MeC<sub>6</sub>H<sub>4</sub>, R<sub>4</sub> = Me, Et) from R<sub>3</sub>NHC(OR<sub>4</sub>):NR<sub>3</sub>.

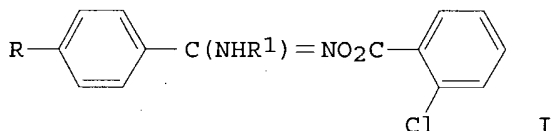
L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1976:542212 CAPLUS  
DOCUMENT NUMBER: 85:142212  
TITLE: Elimination reactions with anilide oxime  
o-chlorobenzoates: rearrangement into carbodiimides  
by reaction with sodium tert-amylate  
AUTHOR(S): Garapon, Jacques; Sillion, Bernard  
CORPORATE SOURCE: Inst. Fr. Pet., CEN, Grenoble, Fr.  
SOURCE: Bulletin de la Societe Chimique de France (1975),  
(11-12, Pt. 2), 2671-6  
CODEN: BSCFAS; ISSN: 0037-8968

09/759,633

DOCUMENT TYPE: Journal  
LANGUAGE: French  
OTHER SOURCE(S): CASREACT 85:142212  
IT 57767-04-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of)  
RN 57767-04-1 CAPLUS  
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)



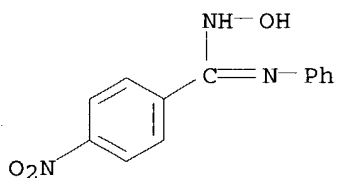
GI



AB The elimination reaction of I (R = H, p-MeO, p-NO<sub>2</sub>; R<sup>1</sup> = Ph, cyclohexyl, 2,6-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>) with sodium tert-amylate occurred via a carbodiimide intermediate. A concerted reaction mechanism was postulated.

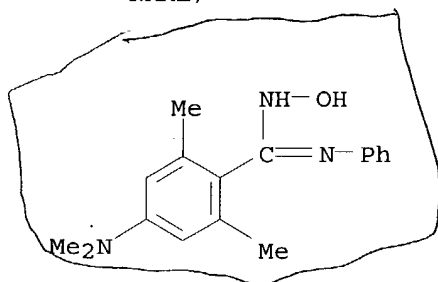
L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1975:592705 CAPLUS  
DOCUMENT NUMBER: 83:192705  
TITLE: Synthetic reactions using transition metal complexes. Conversion of amide oximes into amidines by pentacarbonyliron and evidence for imine intermediates in the deoxygenation of ketoximes  
AUTHOR(S): Dondoni, Alessandro; Barbaro, Gaetano  
CORPORATE SOURCE: Ist. Chim. Org., Univ. Bologna, Bologna, Italy  
SOURCE: Journal of the Chemical Society, Chemical Communications (1975), (18), 761-2  
CODEN: JCCCAT; ISSN: 0022-4936  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 83:192705  
IT 57767-04-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reductive dehydroxylation of, by pentacarbonyliron)  
RN 57767-04-1 CAPLUS  
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX NAME)

09/759,633

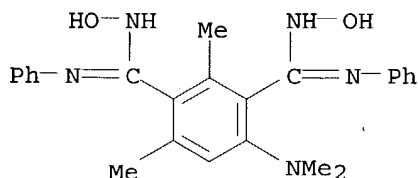


AB Treatment of  $\text{RC}(:\text{NOH})\text{NR}_1\text{R}_2$  ( $\text{R} = \text{Ph}$ ,  $\text{R}_1 = \text{H}$ ,  $\text{R}_2 = \text{Ph}$ ,  $\text{C}_6\text{H}_4\text{Cl-p}$ ;  $\text{R} = \text{Ph}$ ,  $\text{R}_1 = \text{Me}$ ,  $\text{R}_2 = \text{Ph}$ ,  $\text{Me}$ ;  $\text{R} = \text{Mesityl}$ ,  $\text{p-O}_2\text{NC}_6\text{H}_4$ ,  $\text{R}_1 = \text{H}$ ,  $\text{R}_2 = \text{Ph}$ ) with  $\geq 1$  equiv  $\text{Fe}(\text{CO})_5$  in refluxing dry THF gave 70-90%  $\text{RC}(:\text{NH})\text{NR}_1\text{R}_2$ .  
2,4,6-Me $_3\text{C}_6\text{H}_2\text{C}(:\text{NOH})\text{Me}$  reacted similarly.

L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1967:454096 CAPLUS  
DOCUMENT NUMBER: 67:54096  
TITLE: Nitrile oxides. IX. Basic substituted stable nitrile oxides  
AUTHOR(S): Grundmann, Christoph; Richter, Reinhard  
CORPORATE SOURCE: Mellon Inst., Pittsburgh, PA, USA  
SOURCE: Journal of Organic Chemistry (1967), 32(7), 2308-12  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 67:54096  
IT 13012-21-0P 13012-22-1P  
RL: SPN (Synthetic preparation); PREP (Preparation of preparation of)  
RN 13012-21-0 CAPLUS  
CN Benzamidoxime, 4-(dimethylamino)-2,6-dimethyl-N-phenyl- (8CI) (CA INDEX NAME)



RN 13012-22-1 CAPLUS  
CN Isophthalamidoxime, 4-(dimethylamino)-2,6-dimethyl-N,N'-diphenyl- (8CI) (CA INDEX NAME)



AB cf. CA 66: 37812e. Nitrile oxides of the benzene and pyrimidine series, stabilized by controlled steric hindrance and substituted by a Me $_2\text{N}$  group,

are described and some of their reactions discussed. These compds. are the 1st isolated nitrile oxides which contain an addnl. different functional group. 21 references.

L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:431660 CAPLUS

DOCUMENT NUMBER: 63:31660

ORIGINAL REFERENCE NO.: 63:5630f-h,5631a-b

TITLE: Synthesis of 2-oxo-1,2,3,5-oxathiadiazoles

AUTHOR(S): Eloy, F.; Lenaers, R.

CORPORATE SOURCE: Union Carbide European Res. Assoc., Brussels

SOURCE: Bulletin des Societes Chimiques Belges (1965),  
74(3-4), 129-35

CODEN: BSCBAG; ISSN: 0037-9646

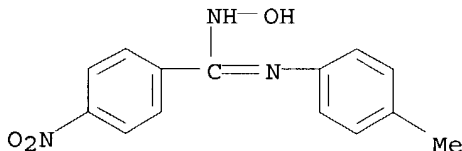
DOCUMENT TYPE: Journal

LANGUAGE: French

IT 2630-07-1, p-Benzotoluidide, 4-nitro-, oxime  
(preparation of)

RN 2630-07-1 CAPLUS

CN Benzenecarboximidamide, N-hydroxy-N'-(4-methylphenyl)-4-nitro- (9CI) (CA  
INDEX NAME)



GI For diagram(s), see printed CA Issue.

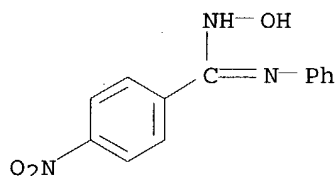
AB A series of derivs. (I) of 2-oxo-1,2,3,5-oxathiadiazole was prepared by the dipolar addition of sulfinylamines to nitrile oxides. I were also formed by treating the appropriate N-substituted amide oxime with SOCl<sub>2</sub> in C<sub>5</sub>H<sub>5</sub>N. p-C<sub>6</sub>H<sub>4</sub>(CNO)<sub>2</sub> (3.2 g.) in 100 cc. dioxane stirred .apprx.12 hrs. with 5.6 g. PhNSO (II) yielded 7.6 g. III, m. 180° (decomposition). p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CCl:NOH (IV) (10 g.) in the min. amount EtOH treated dropwise at -10 to -5° with 6 g. Et<sub>3</sub>N gave 7.8 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CNO (V), m. 95°. V (3.3 g.) and 2.8 g. II added at 10° to 100 cc. dry C<sub>6</sub>H<sub>6</sub> and the mixture kept 2 hrs. at room temperature and refluxed 0.5 hr. yielded

6 g. I (R = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, R<sub>1</sub> = Ph) (VI), m. 140° (C<sub>6</sub>H<sub>6</sub>-hexane). IV (10 g.) and 6.9 g. II in 150 cc. dry C<sub>6</sub>H<sub>6</sub> treated with 5 g. Et<sub>3</sub>N and kept at room temperature overnight gave 4 g. VI, m. 140°. V (1.64 g.) in 50 cc. dry C<sub>6</sub>H<sub>6</sub> treated dropwise with 1.19 g. BuNSO in C<sub>6</sub>H<sub>6</sub> and kept overnight yielded 0.250 g. I (R = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, R<sub>1</sub> = Bu), m. 54° (petr. ether). IV (20 g.) in 100 cc. dry Et<sub>2</sub>O treated with 21.4 g. p-MeC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> in Et<sub>2</sub>O and the mixture kept overnight gave 15.5 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>C(:NOH)NHC<sub>6</sub>H<sub>4</sub>Me-p (VII), m. 186° (aqueous EtOH). VII (7.8 g.) in 100 cc. dry C<sub>6</sub>H<sub>6</sub> containing 6 cc. C<sub>5</sub>H<sub>5</sub>N treated dropwise at 10° with 3.4 g. SOCl<sub>2</sub> and the mixture kept 2 hrs. and heated 1 hr. at 80° gave 9.5 g. I (R = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, R<sub>1</sub> = p-MeC<sub>6</sub>H<sub>4</sub>), m. 120° (C<sub>6</sub>H<sub>6</sub>-hexane). PrNO<sub>2</sub> (26.7 g.) in 1500 cc. dry C<sub>6</sub>H<sub>6</sub>, 72 g. PhNCO, and 42 g. II treated dropwise at 15° with 3 cc. Et<sub>3</sub>N in 20 cc. dry C<sub>6</sub>H<sub>6</sub> and the mixture kept 3 hrs. at room temperature, heated 3 hrs. at 70°, and refrigerated overnight gave 35 g. I (R = Et, R<sub>1</sub> = Ph), m. 78° (hexane). Similarly were prepared I (R = Et, R<sub>1</sub> = p-MeC<sub>6</sub>H<sub>4</sub>), I (R = Et, R<sub>1</sub> = p-ClC<sub>6</sub>H<sub>4</sub>), and I (R = Et, R<sub>1</sub> = p-MeOC<sub>6</sub>H<sub>4</sub>) as oils which could not be

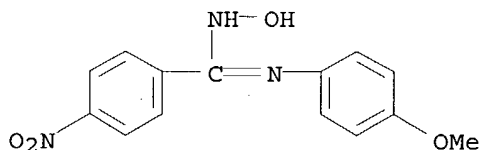
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obtained pure.

L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1962:38478 CAPLUS  
DOCUMENT NUMBER: 56:38478  
ORIGINAL REFERENCE NO.: 56:7304c-h  
TITLE: Decarboxylation of 1,2,4-oxadiazol-5-ones. Syntheses  
of benzimidazoles. II  
AUTHOR(S): Bacchetti, Tullio; Alemagna, Andreina  
CORPORATE SOURCE: Univ. Milan  
SOURCE: Atti Accad. Nazl. Lincei, Rend., Classe Sci. Fis.,  
Mat. e Nat. (1960), 28, 824-35  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
IT 57767-04-1, Benzanilide, 4-nitro-, oxime 96633-78-2,  
p-Benzanisidide, 4-nitro-, oxime  
(preparation of)  
RN 57767-04-1 CAPLUS  
CN Benzenecarboximidamide, N-hydroxy-4-nitro-N'-phenyl- (9CI) (CA INDEX  
NAME)



RN 96633-78-2 CAPLUS  
CN p-Benzanisidide, 4-nitro-, oxime (7CI) (CA INDEX NAME)



AB cf. CA 52, 15511g; 55, 16527a. Substituted benzanilide oximes, ArC(:NOH)NHar', were prepared in 4 ways (A: ArCSNHar' + NH<sub>2</sub>OH; B: ArCN → O + Ar'NH<sub>2</sub>; C: ArCCl:NOH + Ar'NH<sub>2</sub>; D: ArCCl:NAr' + NH<sub>2</sub>OH) and converted with ClCO<sub>2</sub>Et to oxadiazolones. These were decarboxylated by pyrolysis to give in most cases the corresponding benzimidazoles. The following oximes, oxadiazolones, and benzimidazoles were prepared (Ar and Ar', method of preparation, % yield and m.p. of the benzanilide oxime, % yield and m.p. of the corresponding 1,2,4-oxadiazol-5-one, temperature of pyrolysis, and the % yield, name, and m.p. of the product given): Ph, o-MeC<sub>6</sub>H<sub>4</sub>, D, -, -, 86, 148°, 220°, 91.5, 2-phenyl-4methylbenzimidazole (246°); Ph, o-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, D, -, -, 86, 125°, 255°, 78, 2-phenyl-4-nitrobenzimidazole (I), -, -, 86, 125°, 255°, 78, 2-phenyl-5-nitrobenzimidazole (II), m. 203° (60%); Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, D, -, 152°, 85, 125°, 230°, 75, II, 203°; p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Ph, D, 65, 183°, 90, 201°, 220°, 73.5,

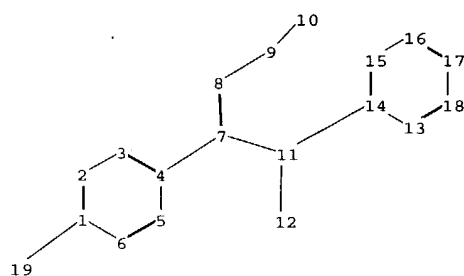
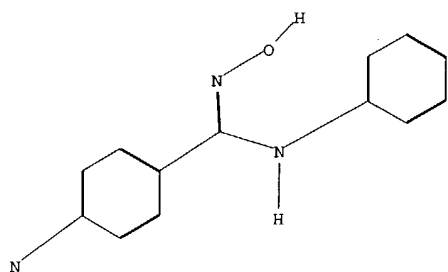
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2-(p-nitrophenyl)benzimidazole, 310°; p-MeOC<sub>6</sub>H<sub>4</sub>, Ph, D, 45, 120-1°, 90, 160°, 190°, 14, 2-(p-methoxyphenyl)benzimidazole. 227°; p-MeOC<sub>6</sub>H<sub>4</sub>, m-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>. D, -, 135°, 75, 173°, 190°, 28, 2-(p-methoxyphenyl)-4 (and 5)-nitrobenzimidazole, 228-33°; Ph, β-naphthyl, D, 80, 182°, 91, 181°, 220°, 71, 2-phenyl-α (or β)-naphthimidazole (III), -. Ph, α-naphthyl, B, 90, 177°, 89, 141°, 250°, 26.5, III, -. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, p-MeOC<sub>6</sub>H<sub>4</sub>, D, 70, 163°, 88, 172°, 220°, -, -, -; Ph, p-EtOC<sub>6</sub>H<sub>4</sub>, B, 65, 157°, 88, 138°, 250°, -, -, -; Ph, β-pyridyl, A, -, 188°, 50, 168°, 180°, -, -, -.

Two bis(oxadiazolones) were obtained. Oxanilide dioxime refluxed 12 hrs. in dioxane (IV) with ClCO<sub>2</sub>Et, the precipitate washed with H<sub>2</sub>O and crystallized from IV

yielded 3,3'-bis(4-phenyl-1,2,4-oxadiazol-5-one), m. 265°. Preparation by method C gave 71% oxalo-p-toluidide dioxime (V), m. 201°. V treated in IV with ClCO<sub>2</sub>Et gave 68% 3,3'-bis(4-p-tolyl-1,2,4-oxadiazol-5-one) m. 261°. Benzanilide oxime (VI) rearranged with PCl<sub>5</sub> in Et<sub>2</sub>O to PhNHCONHPh. Pyrolysis of VI at 165-200° yielded a small amount of 2-phenylbenzimidazole.





chain nodes :

7 8 9 10 11 12 19

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

1-19 4-7 7-8 7-11 8-9 9-10 11-12 11-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-19 7-8 7-11 8-9 11-14

exact bonds :

4-7 9-10 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems :

containing 1 : 13 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS